

PROJECT NUMBER: 1752
PROJECT TITLE : Optical Spectroscopy of Tobacco and Smoke
PROJECT LEADER: R. A. Fenner
PERIOD COVERED: September, 1985

I. HYDROGEN BONDING STUDY OF PYRAZINE-ETHANOLS

Two series of pyrazine-ethanols being investigated by Y. Houminer as pyrolytic flavor release agents were evaluated for "free" and intramolecularly hydrogen bonded hydroxyl content by infrared transmission spectroscopy. The spectra obtained for the compounds were subjected to a band-fitting analysis to establish the relative proportions of "free" and "bonded" hydroxyl. The results suggest there is an inverse relationship between pyrolysis rates and the proportion of "bonded" hydroxyl when steric effects (of substituents) are the dominate factor controlling intramolecular hydrogen bonding. When electronic as well as steric factors influence the proportion of "bonded" versus "free" hydroxyl, the correlation with pyrolysis rates becomes more difficult to define.

II. NICOLET 60 SX GC/FT-IR SYSTEM

Problems encountered with system crashes appear to have been eliminated by a complete replacement of the Nicolet computer system. Spurious software handups during GC data collection are still being addressed by programmers at Nicolet. An investigation is currently in progress to evaluate (for Rett Southwick and Dick Howe) products from reactions involving anhydroscclareodiol and related systems by GC/FT-IR.

III. SIDESTREAM SMOKE ANALYSIS BY TUNABLE DIODE LASER (TDL)

An optical configuration and sampling system have been setup for sidestream smoke analysis. Initial work has focused on water in sidestream. From preliminary studies, the amount of water vapor measured does not appear to depend on the presence of aerosol since sidestream smoke filtered with a Cambridge pad gives the same amount of water vapor (by TDL analysis) as unfiltered smoke. This independence may arise from a cooling of the aerosol (reduced volatilization) as it enters the low pressure, <15 torr, sample cell.

IV. DETERMINATION OF TOTAL AMMONIA RELEASE DURING CURING

Total ammonia was determined on the curing chamber atmosphere during curing of bright tobacco under normal conditions and under high humidity conditions. Maximum ammonia values were observed during the fourth day of curing for both conditions. There was some difference in the magnitude of ammonia for the two conditions which cannot be explained at this time.

V. MEMOS

- A. "Preliminary Studies - Ammonia/Menthol", M. E. Parrish to R. H. Cox, September 5, 1985.
- B. "Hydrogen Bonding Study of Pyrazine - Ethanols", R. A. Fenner to Dr. Y. Houminer, September 25, 1985.

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